3D Phase Images of Lead Nanocrystals

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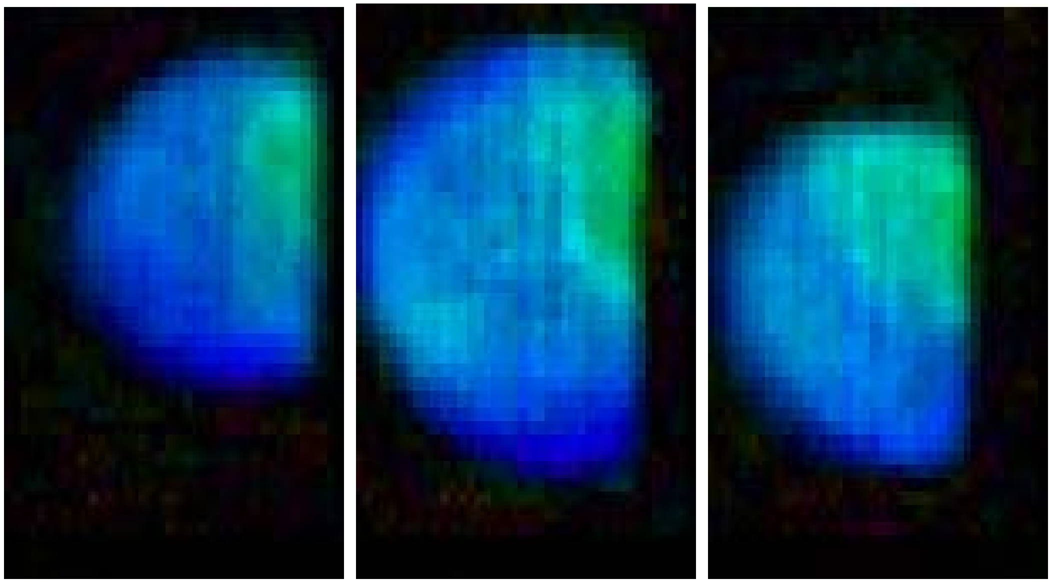

- 500nm Pb crystals grown in-situ in UHV system at APS (Argonne) on a SiO_2 support (vertical).
- 3D coherent X-ray diffraction data is inverted into hemi-spherical cross-sectional slices.

- These images are colored according to the phase of the density, which changes abruptly at an internal boundary.
- This plane is identified as a single deformation fault in the crystal.

The new method used to obtain these images is being developed under the term of the current NSF grant. Diffraction from crystal lattices by electrons or X-rays is sensitive to the structure at the atomic level, but suffers from the problem that only the amplitude (square root of intensity) can be measured and the phase of the wave is lost. The desired information is the complex Fourier transform of the image density, which requires both amplitude and phase. We use computational methods to recover this lost phase, taking advantage of the analytical properties of the Fourier transform: if the amplitude function is sufficiently oversampled, its phase information is also embedded and can be recovered by an appropriate computational algorithm. The oversampling of the diffraction is possible whenever it is continuous and not broken into discrete Bragg spots, as for a large (infinite) crystal. A small nanocrystal has a continuous diffraction pattern which can be measured at the coherent X-ray diffraction facility we built at Argonne, with NSF MRI funds (grant DMR-9724294). In simple cases, the density function is a real quantity which leads to a symmetric diffraction pattern, but small deviations from symmetry are always seen in practice. Here the density is allowed to become complex and shows up as a phase in real space that is mapped as color in the images shown. A straightforward explanation of the origin of the phase boundary is a single deformation fault in the crystal that shifts the atoms on one side with respect to those on the other.

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- Educational Impact
  - Two graduate students, Mark Pfeiffer and Garth Williams performed these experiments and had the original idea of allowing to vary the phase of the object.
  - They are about to start postoc positions where they will transfer their new knowledge of inverting diffraction to other groups.

- Broader Impact
  - This is the first meaningful example of inversion of diffraction from a phase object.
  - Once it is published prominently, the method will be widely applicable to the study strain fields around dislocations, quantum dots and elsewhere.